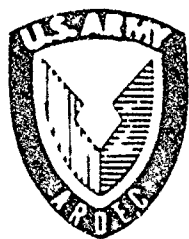②

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DIFFRACTION MODELS, DYNAMICAL STRUCTURE TENSORS, AND ELECTRON-PHONON INTERACTION

L. V. MEISEL

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A coherent exposition of the theory of scattering from a dynamic lattice, which applies to the scattering of Bloch wave electrons as well as to the scattering of plane waves, is presented. This is achieved by developing a generalized diffraction model, along the lines conceived by Van Hove, appropriate for the scattering of Bloch waves. The resulting diffraction model provides a basis for treating processes controlled by electron-phonon interaction in general and subsumes the standard diffraction model results.

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20. ABSTRACT (CONT'D)

The diffraction model origins of the standard approximate expressions
used to describe electron-phonon interaction controlled processes are
also revealed.

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INTRODUCTION

The diffraction model allows for a consistent treatment of diverse scattering phenomena. For example, when electron-phonon interaction is the scattering mechanism, the diffraction model provides a unified treatment of electrical and thermal transport; phonon contributions to the electron effective mass; and acoustic attenuation in perfect and point- or line-defected crystalline alloys, and also in liquid, amorphous, and disordered alloys.

The essence of diffraction model methods is the factorization of scattering rate matrix elements into terms such that the lattice vibrational properties are entirely contained in dynamical structure factors, which can be related to transforms of generalized pair distribution functions.

The most celebrated dynamical structure factor is that defined by Van Hove (ref 1), viz.,

$$S(K,\Omega) = \int_{-\infty}^{\infty} dt \exp(i\Omega t) < r(K,t)r^+(K,0) >_T \qquad (1)$$

where $<O>_T$ denotes thermal average in the equilibrium ensemble (i.e., $<O>_T = \Sigma \, p_i <i| \, O \, | i>$), and $r(K,t)$ is the spatial Fourier transform of the ion density operator. The Van Hove dynamical structure factor $S(K,\Omega)$ describes very general scattering phenomena in which the lattice absorbs pseudo-momentum K and energy Ω. It is directly measurable via neutron scattering experiments. It encompasses Debye-Waller factors, umklapp processes, couplings to transverse phonons, multiphonon effects, etc. Thus, $S(K,\Omega)$ has been the object of intense theoretical interest.

Baym (ref 2) elaborated a diffraction model approach to the treatment of electron-phonon interaction controlled phenomena based upon the Van Hove dynamical structure factor. Baym's approach has proven to be extremely productive and has become standard. However, Baym's form of the diffraction model, based on

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the Van Hove dynamical structure factor, is strictly correct only for the scattering of plane (or pseudoplane) waves (PWs). To apply diffraction model techniques to electron-phonon interaction controlled processes in general, it is necessary to derive diffraction model expressions appropriate for treating the scattering of Bloch waves (BWs).

Therefore, the principal objective of this report is to present a coherent exposition of a generalized diffraction model which applies to PWs or BWs in perfect, disordered, or defected crystalline alloys and to PWs in liquid or amorphous alloys. This aim is realized through the introduction of a generalized diffraction model which applies to BW electron-phonon interaction controlled processes and reduces to the standard diffraction model in PW scattering cases.

An important secondary objective is to reveal the diffraction model origins of the approximate expressions appearing in the standard literature. In particular, the standard equations used to describe electron-phonon interaction controlled processes are approximate diffraction model expressions.

THE GENERALIZED DIFFRACTION MODEL

The development of diffraction model factorizations for scattering of BWs is demonstrated in this section. The essential diffraction model ideas are contained in Reference 1. The theoretical development follows that presented in Reference 3. The methods employed here were also used by Van Hove (ref 1). The crucial step in either reference is the application of Bloch's Theorem (ref 4).

In order to streamline the notation: (1) Let q stand for (q,j) where q is a phonon wave vector and j is a phonon branch and polarization index. (2) Let k stand for (k,s) where k is the scattered particle wave vector and s is an

appropriate index. For example, for electron states, s might represent the

spin. (3) Consider pure materials. (The generalization required to treat

alloys, via the introduction of partial structure factors, is straightforward

and well known.) (4) The following shorthand notations are adopted:

$$K = k - k', \quad A = K + G - H, \quad \text{and} \quad A' = K + G' - H'$$

where G, H, G', and H' are reciprocal lattice vectors (RLVs).

Scattering from an initial state containing a BW of wave number index k,

$$|k,i\rangle = \sum_G \alpha(G) \exp[i(k+G).x] \, |i\rangle \tag{2a}$$

into a final state containing a BW of wave number index k',

$$|k',f\rangle = \sum_G \beta(G) \exp[i(k'+G).x] \, |f\rangle \tag{2b}$$

is treated. The sums are on RLV G.

The perturbation H' producing the scattering is assumed to be of the form

$$H' = \sum_l [V(x-x_l) - U(x-l)] \tag{3}$$

where x_l is the position of the ion, which, in the absence of the lattice vibra-

tion, would be at position l, V(x) is the ionic potential, and U(x) is the

unperturbed potential. We think of these potentials as fully screened, etc.,

and use the same letters to denote the Fourier transforms,

$$\{U(A),V(A)\} = \int dx \, \exp[iA.x]\{U(x),V(x)\} \tag{4a}$$

The origin is chosen in such a way that

$$A.l = K.l + (\text{integer})2\pi$$

We also denote the difference in the transformed potentials (i.e., the transform

of the undisplaced potentials) by

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$$W(A) = V(A) - U(A) \tag{4b}$$

Thus, using Eqs. (2) to (4),

$$\langle k',f| H'| k,i\rangle = \sum_{l,G,H} \beta(G){*}\alpha(H)\{V(A)\langle f| \exp[iA.x_l]| i\rangle -U(A)\exp[iK.l]\langle f| i\rangle\} \tag{5}$$

and

$$\langle k',f| H'| k,i\rangle\exp[i(\epsilon_i-\epsilon_f)] = \sum_{l,G,H} \beta(G){*}\alpha(H)\{V(A)\langle f| \exp[iA{\cdot}x_l(t)]| i\rangle$$

$$-U(A)\exp[iK.l]\langle f| i\rangle\} \tag{6a}$$

where $x_l(t)$ is in Heisenberg representation and we have used

$$H_0| i\rangle = \epsilon_i| i\rangle \tag{6b}$$

and

$$H_0| f\rangle = \epsilon_f| f\rangle \tag{6c}$$

It then follows that the scattering rate, neglecting factors accounting for occupation of the states k, k', etc., is given by

$$X(k,k',\Omega) = \sum_{i,f} p_i \, | \langle k',f| H'| k,i\rangle|^2 \, \delta(\epsilon_i-\epsilon_f-\Omega)$$

$$= \sum_{i,f} \int \frac{dt}{2\pi} p_i \, | \langle \kappa',f| H'| k,i\rangle|^2 \, \exp[i(\epsilon_i-\epsilon_f-\Omega)t]$$

$$= \sum_{G,H.G',H'} \beta(G){*}\alpha(H)[\beta(G'){*}\alpha(H')]{*}$$

$$\{V(A)V(A'){*}S'(A,A'.\Omega) + W(A)W(A'){*}a(K)\delta(\Omega)\} \tag{7}$$

where the geometrical structure factor a(K) is defined in the usual way, i.e.,

$$a(K) = \sum_{l,l'} \exp[iK.(l-l')] = N \sum_{d} \exp[iK.d] \tag{8}$$

The dynamical structure factor $S'(A,A',\Omega)$ is defined as

$$S'(A,A',\Omega) = S(A,A',\Omega) - a(K)\delta(\Omega) \qquad (9a)$$

where the dynamical structure factor $S(A,A',\Omega)$ is defined as

$$S(A,A',\Omega) = \sum_{l,l'} \exp[iK.(l-l')]$$

$$\int \frac{dt}{2\pi} \exp[-i\Omega t] \langle \exp[-iA'.u_{l'}(0)]\exp[iA.u_l(t)]\rangle_T \qquad (9b)$$

and $u_l(t)$ is the displacement of the ion at l due to the lattice vibrations, i.e., $x_l(t) = l + u_l(t)$. Note that Eq. (7) allows for arbitrary combinations of disorder and defect scattering; for example, Eq. (7) allows for straightforward application to scattering in impure and/or point defect containing crystalline solids at finite temperature.

$S(A,A',\Omega)$ is a generalization of the Van Hove dynamical structure factor (ref 1), i.e.,

$$S(K,K,\Omega) = S(K,\Omega) \qquad (9c)$$

and $S'(A,A',\Omega)$ is a generalization of the modified Van Hove dynamical structure factor, defined by Baym (ref 2), i.e.,

$$S'(K,K,\Omega) = S'(K,\Omega) \qquad (9d)$$

Generalizing the development in Reference 3, one obtains

$$\langle \exp[-iA'.u_{l'}(0)]\exp[iA.u_l(t)]\rangle_T = \exp[A'.Z(l-l',t).A] \qquad (10a)$$

where

$$Z(d,t) = - \sum_q W_q \left(\langle 2n_q+1\rangle - \langle n_q+1\rangle\exp[i\theta_{d,t}] - \langle n_q\rangle\exp[-i\theta_{d,t}] \right) \qquad (10b)$$

where

$$W_q = e_q e_q/2NM\Omega_q \qquad (10c)$$

and $d = 1-1'$ is an ion spacing in the absence of thermal vibrations; N is the number of ions; M the ion mass; Ω_q, n_q, and e_q are the phonon frequency, number density, and polarization vector at q, respectively, and

$$\theta_{d,t} = q.d + \Omega_q t \qquad (10d)$$

Note that $Z(d,t)$ is a symmetric second rank tensor which is independent of K, A, and A'.

Thus, we can express the dynamical structure factor $S(A,A',\Omega)$ in the form

$$S(A,A',\Omega) = N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]\exp[A.Z(d,t).A'] \qquad (11a)$$

$$= \sum_{n=0} [A.. .A].. .I_n(K,\Omega).. .[A'.. .A']/n! \qquad (11b)$$

where $[A.. .A]$ is an n-fold open product of the vector A. Equation (11b) defines the structure tensor $I_n(K,\Omega)$ of rank 2n and is obtained by expanding the exponential in Eq. (11a) and performing the sum over d and the t integration. (N.B., the tensor $I_n(K,\Omega)$ is not uniquely defined by Eq. (11b); however, the most symmetric forms with respect to the left and right inner products are the obvious choice and are intended.)

Combining Eqs. (7) and (11),

$$X(k,k',\Omega) = \sum_{G,H,G',H'} \beta(G)*\alpha(H)[\beta(G')*\alpha(H')]*$$

$$(V(A)V(A')*S'(A,A',\Omega) + W(A)W(A')*a(k)\delta(\Omega))$$

$$= \sum_{n=1} V_n(k,k')*.. .I_n(K,\Omega).. .V_n(k,k')/n! + |W_0(k,k')|^2 I_0(K,\Omega) \qquad (12)$$

where we have defined the scalar

$$W_0(k,k') = \langle k'| W(x) | k \rangle \tag{13a}$$

and for n=1 to ∞, the rank n tensor

$$V_n(k,k') = \langle k'| \{[(i\nabla)\dots(i\nabla)]V(x)\} | k \rangle \tag{13b}$$

and we have used the relation

$$\sum_{G,H} \beta(G)^*\alpha(H) [A\dots A]V(A) = \int dx \{\sum_H \beta(H)\exp[i(k'+H).x]\}^*$$

$$\{[(i\nabla)\dots(i\nabla)]V(x)\}\{\sum_G \beta(G)\exp[i(k'+G).x]\}$$

$$= \langle k'| \{[(i\nabla)\dots(i\nabla)]V(x)\} | k \rangle = V_n(K) \tag{13c}$$

All the dynamical properties of the lattice are contained in the structure tensors $\{I_n(K,\Omega) | n=0, \infty\}$.

Equation (12), with $\{I_n(K,\Omega) | n=0, \infty\}$ defined in Eqs. (10) and (11), $W_0(k,k')$ defined in Eq. (13a), and the $\{V_n(k,k') | n=1,\infty\}$ defined in Eq. (13b), constitute the generalized diffraction model expression and are the principal results of this report. N.B., to obtain actual scattering rates, one must include appropriate factors (e.g., $(2\pi/h)f(k)[1-f(k')]$) in Eq. (12).

PLANE WAVE SCATTERING, n-PHONON STRUCTURE TENSOR $\Phi_n(K,\Omega)$, DEBYE-WALLER TENSOR W, AND THE VAN HOVE DYNAMICAL STRUCTURE FACTOR $S(K,\Omega)$

Since the first term in Eq. (10b) is independent of d and t, it is useful to define the tensor

$$Z'(d,t) = \sum_q w_q [\langle n_q+1\rangle\exp(i\theta_{d,t})+\langle n_q\rangle\exp(-i\theta_{d,t})] \tag{14a}$$

and

$$W = \sum_q w_q \langle 2n_q+1\rangle \tag{14b}$$

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Thus, Eq. (10b) can be rewritten in the form

$$Z(d,t) = -W + Z'(d,t) \qquad (14c)$$

and since the Debye-Waller exponent $2W(K)$ is simply related to W, viz.,

$$2W(K) = K.W.K \qquad (14d)$$

we designate W as the (second rank) Debye-Waller tensor.

Equations (14a) through (14d) suggest that a different factorization of the scattering rate will be particularly appropriate in the PW case. The treatment of PW scattering leads in a natural way to the introduction of n-phonon structure tensors $\{\Phi_n(K,\Omega)\}$, which are also useful in expressing limiting BW expressions. Thus, Eq. (2a) becomes

$$|k,i\rangle = \exp[ik.x] \, |i\rangle \qquad (15a)$$

etc., and

$$A,A' \longrightarrow K \qquad (15b)$$

Thus, recalling Eq. (9), Eq. (11) yields

$$S(K,\Omega) = N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]\exp[K.Z(d,t).K] \qquad (16a)$$

$$= \sum_{n=0} [K...K]... \, .I_n(K,\Omega)... \, .[K...K]/n! \qquad (16b)$$

Employing Eqs. (14c) and (14d), Eq. (16a) yields

$$S(K,\Omega)=\exp[-2W(K)] \, N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]\exp[K.Z'(d,t).K]$$

$$= \exp[-2W(K)] \sum_{n=0} [K.. \, .K].. \, .\Phi_n(K,\Omega).. \, .[K.. \, .K]/n! \qquad (16c)$$

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Equations (14a) and (16c) define $\{\Phi_n(K,\Omega)\}$, which are designated as the n-phonon structure tensors and $\exp[-2W(K)](=\exp[-K.W.K])$ is the Debye-Waller factor. (We can also relate the $\{I_n(K,\Omega)\}$ to the $\{\Phi_n(K,\Omega)\}$ by expanding $\exp[-2W(K)]$, forming the product, and identifying the tensor coefficients.)

THE LOW ORDER STRUCTURE TENSORS

Since the structure tensors play a central role in diffraction models, it is worthwhile to display the expressions for the first few in some detail. The expressions are deduced by examination of expansions in Eq. (16).

The Zero Rank Structure Tensor $I_0(K,\Omega)$ and 0-Phonon Structure Tensor $\Phi_0(K,\Omega)$

$$\Phi_0(K,\Omega) = I_0(K,\Omega) = N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t] = a(K)\delta(\Omega) \qquad (17)$$

defines the zero rank structure tensor $I_0(K,\Omega)$ and zero rank 0-phonon structure tensor $\Phi_0(K,\Omega)$.

The Second Rank Structure Tensor $I_1(K,\Omega)$ and 1-Phonon Structure Tensor $\Phi_1(K,\Omega)$

$$I_1(K,\Omega) = N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t] \, Z(d,t)$$

$$= N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]$$

$$\sum_q w_q \left[-<2n_q+1> + <n_q+1>\exp(i\theta_{d,t}) + <n_q>\exp(-i\theta_{d,t}) \right]$$

$$= -a(K)\delta(\Omega)W + \Phi_1(K,\Omega) = I_0(K,\Omega)(-W) + \Phi_1(K,\Omega) \qquad (18a)$$

where

$$\Phi_1(K,\Omega) = \sum_q w_q \left[<n_q+1>a(K+q)\delta(\Omega-\Omega_q) + <n_q>a(K-q)\delta(\Omega+\Omega q) \right] \qquad (18b)$$

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is the 1-phonon scattering structure tensor, Eq. (14b) defines the (second rank) Debye-Waller tensor W, and we have used

$$a(K \pm q)\delta(-\Omega \pm \Omega_q) = \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]\exp(\pm i\theta_{d,t}) \qquad (18c)$$

The Fourth Rank Structure Tensor $I_2(K,\Omega)$ and 2-Phonon Structure Tensor $\Phi_2(K,\Omega)$

$$I_2(K,\Omega)_{i,i',h',h} = N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t] Z(d,t)_{i,h} \, Z(d,t)_{i',h'}$$

$$= N \sum_d \exp[iK.d] \int \frac{dt}{2\pi} \exp[-i\Omega t]$$

$$\sum_{q'} [w_{q'}]_{i',h'}[<2n_{q'}+1> - <n_{q'}+1>\exp(i\theta'_{d,t}) - <n_{q'}>\exp(-i\theta'_{d,t})]$$

$$\sum_{q} [w_q]_{i,h} [<2n_q+1> - <n_q+1>\exp(i\theta_{d,t}) - <n_q>\exp(-i\theta_{d,t})]$$

$$= a(K)\delta(\Omega)[W_2]_{i,i',h',h} - [W]_{i,h} [\Phi_1(K,\Omega)]_{i',h'}$$

$$- [\Phi_1(K,\Omega)]_{i,h} [W]_{i',h'} + [\Phi_2(K,\Omega)]_{i,i';h',h} \qquad (19a)$$

where

$$\Phi_2(K,\Omega) = \sum_{q,q'} \Gamma_{q,q'} \, (<n_q+1><n_{q'}+1>a(K+q+q')\delta(\Omega-\Omega_q-\Omega_{q'})$$

$$+<n_q+1><n_{q'}>a(K+q-q')\delta(\Omega-\Omega_q+\Omega_{q'})$$

$$+<n_q><n_{q'}+1>a(K-q+q')\delta(\Omega+\Omega_q-\Omega_{q'})$$

$$+<n_q><n_{q'}>a(K-q-q')\delta(\Omega+\Omega_q+\Omega_{q'})) \qquad (19b)$$

is designated as the 2-phonon scattering structure tensor,

$$\Gamma_{q,q'} = e_{q'}e_q e_q e_{q'}/[(2NM)^2 \, \Omega_q \Omega_{q'}] \tag{19c}$$

and

$$[W_2]_{i,i',h',h} = W_{i,h}W_{i'h'} \tag{19d}$$

where $W_{i,h}$ is the i,h component of the Debye-Waller tensor. (One might designate $[W_2]_{i,i',h',h}$ as the fourth rank Debye-Waller tensor.)

EXPERIMENTAL EVALUATION OF $S(K,\Omega)$, $I_n(K,\Omega)$, W, AND $\Phi_n(K,\Omega)$

As is well known, $S(K,\Omega)$ may be directly determined by neutron scattering experiments. It is also clear that, in principle, one may deduce the tensor $I_n(K,\Omega)$ from analysis of the expression for $S(K,\Omega)$ contained in Eq. (16b). Similarly one could deduce W and $\{\Phi_n(K,\Omega)\}$ from analysis of the expression for $S(K,\Omega)$ contained in Eq. (16c) or from $\{I_n(K,\Omega)\}$. Of course, in practice the experimental determination of $S(K,\Omega)$ is exacting and the experimental evaluation of $I_n(K,\Omega)$ or $\Phi_n(K,\Omega)$ for n>1 may be impractical. Nevertheless, it is important to note that the same tensors $I_n(K,\Omega)$ or W and $\Phi_n(K,\Omega)$ appear in the BW expression and in the PW expression and that, in principle, one can deduce the tensors appropriate for treating the BW case from the analysis of PW scattering experiments.

THE STANDARD EXPRESSIONS

PW Cases

The standard form: electron scattering in liquid and amorphous metals and neutron scattering

When PWs are appropriate basis functions, Eqs. (15a) and (15b) are appropriate and the two forms, Eqs. (16b) and (16c), define the appropriate structure factor, i.e., the Van Hove dynamical structure factor (ref 1). Furthermore, when a PW basis is employed vanishing unperturbed potential, $(U(x) = 0)$ is appropriate, and thus,

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$$W_0(k,k') = V_0(k,k') \longrightarrow V(K) \tag{20a}$$

Also, recalling Eq. (13)

$$V_n(k,k') = [AA...A]V(k,k') \longrightarrow [KK...K]V(K) = V_n(K) \tag{20b}$$

so that, employing Eqs. (20) and (16b), Eq. (12) becomes

$$X(K,\Omega) = X(k,k',\Omega)$$

$$= \sum_{n=1} V_n(k,k')^*.. .I_n(K,\Omega).. V_n(k,k')/n! + |W_0(k,k')|^2 I_0(K,\Omega)$$

$$= |V(K)|^2 \left\{ \sum_{n=1} [KK...K].. .I_n(K,\Omega).. .[KK...K]/n! + I_0(K,\Omega) \right\}$$

$$= |V(K)|^2 S(K,\Omega) \tag{21}$$

Equation (21) is immediately recognized as the standard form for electron scattering in liquid and amorphous metals and neutron scattering. That is, as they must, the BW expressions reduce to the standard forms in the special case of PWs.

Approximate forms

The approximate forms are based on Eq. (16c) for PWs.

Markowitz's approximation - Markowitz (ref 5) observed that the temperature variation of the electrical resistivity of relatively high resistivity amorphous metals could be reasonably represented by neglecting all but the elastic scattering term in the expression for $S(K,\Omega)$, i.e.,

$$S(K,\Omega) \approx \exp[-2W(K)] \, \Phi_0(K,\Omega) \tag{22}$$

where $\Phi_0(K,\Omega)$ is defined in Eq. (17). (Generalization for anisotropic materials is obvious.) The fact that such a drastic approximation yields reasonable agreement with experiment suggests a breakdown of conventional theory of electrical transport in the relatively high resistivity amorphous metals studied.

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Sham-Ziman approximation - The Sham-Ziman (ref 6) approach to approximating

the multiphonon contributions to the scattering rate is the most popular.

Reference 6 presents arguments to support this procedure, but the simplicity of

the resulting forms and their relatively good performance is at the core of

their wide acceptance. One assumes that the effect of the multiphonon series is

to cancel the effect of the Debye-Waller factor in the 1-phonon term in Eq.

(16c), i.e.,

$$S(K,\Omega) \approx \exp[-2W(K)] \, \Phi_0(K,\Omega) + K \cdot \Phi_1(K,\Omega) \cdot K \tag{23a}$$

where $\Phi_0(K,\Omega)$ and $\Phi_1(K,\Omega)$ are defined in Eqs. (17) and (18b). For isotropic

materials (e.g., amorphous metals), Eq. (23a) becomes

$$S(K,\Omega) \approx \exp[-2W(K)] \, \Phi_0(K,\Omega) + \Phi_1(K,\Omega)K^2 \tag{23b}$$

Other approximations - Other approximations are employed. Sometimes the

multiphonon contributions are simply ignored. Meisel and Cote (ref 7) have com-

pared an approximation proposed by Hernandez-Calderon et al. (ref 8) with the

Sham-Ziman approximation (ref 6). Little basis for selection of one over the

other could be found in fitting experimental data.

Baym's Form: The Nearly Free Electron (NFE) Case

Here we consider an important special case of PW scattering. Strictly

speaking PWs are not appropriate electron basis functions for the treatment of

crystalline materials. Nevertheless, PWs are frequently a reasonable approxima-

tion. We shall refer to such instances as NFE cases.

The NFE procedure for treating scattering of electrons due to lattice

vibrations in perfectly crystalline solids is to use PWs as approximate basis

functions of the unperturbed Hamiltonian H_0, which has a potential of the form,

$$\sum_l U(x-l) \tag{24}$$

where $V(x) = U(x)$. Thus, $W(K) = 0$, and Eq. (13) becomes

$$X(k,k',\Omega) = \sum_{n=1} V_n(k,k')*.. .I_n(K,\Omega).. .V_n(k,k')/n! \qquad (25a)$$

$$= |V(K)|^2 (\sum_{n=1} [KK...K].. .I_n(K,\Omega).. .[KK...K]/n! \qquad (25b)$$

$$= |V(K)|^2 S'(K,\Omega) \qquad (25c)$$

where one uses

$$V_n(k,k') \approx V_n(K) = [K.. .K]V(K) \qquad (25d)$$

which holds for PWs. Note that the elastic term (n = 0) is absent from Eq. (25). Equation (25) is frequently applied in crystalline metals (e.g., Reference 2); we refer to this form as Baym's approximation or the NFE approximation.

Bloch Wave Scattering in Perfect Crystals

The standard form

The procedure for treating scattering of electrons due to lattice vibrations in perfectly crystalline solids (for which an NFE model is inadequate) is to use (approximate) BW solutions of the unperturbed Hamiltonian H_0 as basis functions, where H_0 has a potential of the form,

$$\sum_1 U(x-1) \qquad (26)$$

where $V(x) = U(x)$. Thus, $W(K) = 0$, and Eq. (13) becomes

$$X(k,k',\Omega) = \sum_{n=1} V_n(k,k')*.. .I_n(K,\Omega).. .V_n(k,k')/n! \qquad (27)$$

Note that Eqs. (26) and (27) are identical to Eqs. (24) and (25a); however, since Eq. (25d) does not apply to BWs, the forms in Eqs. (25b) and (25c) do not

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apply to BWs. As in Baym's approximation, the elastic term (n = 0) is absent

from Eq. (27); i.e., the "natural" Bloch electrons are not elastically scattered

in perfect crystals. Equation (23) is the appropriate form to substitute for

$a(K)$ in the expressions for $I_n(K,\Omega)$ in the perfect crystal case.

Approximate forms: Sham-Ziman approximation

The Sham-Ziman approximation (ref 6) was originally introduced in the con-

text of perfect crystals. · The Sham-Ziman approximation for BW scattering yields

$$X(k,k',\Omega) \approx V_1(k,k')^* \cdot \Phi_1(K,\Omega) \cdot V_1(k,k') \tag{28}$$

Thus, substituting Eq. (23) for $a(K)$, one finds

$$X(k,k',\Omega) = \frac{(2\pi)^3}{V_c} \sum_{G,q} \frac{|e_q \cdot V_1(k,k')|^2}{2M\Omega_q} \{<n_q+1>\delta(K+G+q)\delta(\Omega-\Omega_q)$$

$$-<n_q>\delta(K+G-q)\delta(\Omega+\Omega_q)\} \tag{29a}$$

$$=[(2\pi)^3/V_c] \sum_{G,q} |g(k,k')|^2 \{<n_q+1>\delta(K+G+q)\delta(\Omega-\Omega_q)$$

$$-<n_q>\delta(K+G-q)\delta(\Omega+\Omega_q)\} \tag{29b}$$

Equation (29) is in the form usually employed to treat electron-phonon interac-

tion controlled scattering of Bloch electrons in crystalline metals. That is,

the typical study of electron-phonon interaction controlled processes employing

BW electrons implicitly assumes perfect crystallinity and invokes the Sham-Ziman

approximation. For example, Eq. (29) gives the "first principles" form used in

the work of Butler, Pinski, and Allen (ref 9). (One assumes that in Reference

9, $\delta(K-q)$ stands for a summation over RLV G on $\delta(K+G-q)$.) Thus, the diffraction

model origin and the nature of the multiphonon scattering approximation implic-

itly adopted in standard treatments of electron-phonon interaction controlled

processes is revealed.

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ELECTRON-PHONON SPECTRAL FUNCTIONS AND STATIC STRUCTURE FACTORS

When dealing with electron-phonon interaction controlled phenomena, it is customary to define various electron-phonon spectral functions, denoted $\alpha^2(\Omega)F(\Omega)$. For example, the Eliashberg function (ref 10) is an electron-phonon spectral function. The $\alpha^2(\Omega)F(\Omega)$ may be defined by integrating appropriately weighted diffraction model scattering rates over K. These electron-phonon spectral functions are of theoretical importance; however, the procedures followed in applying them often obscure the diffraction model origins of the analyses.

On the other hand, when dealing with electron-phonon interaction controlled phenomena, it is also possible to define static structure factors, which would be denoted $S(K)$, $I_m(K)$, or $\Phi_m(K)$. The various static structure factors (or tensors) may be defined by integrating appropriately weighted diffraction model scattering rates over Ω. The x-ray and resistivity static structure factors for amorphous metals, as discussed by Meisel and Cote (ref 11), are examples. The static structure factors, which are wholly determined by the lattice dynamics, are also of theoretical interest and emphasize the diffraction model origins of the analysis being performed.

CONCLUDING REMARKS

A generalized diffraction model appropriate for BW electrons as well as PW scattering from a dynamic lattice has been presented. It is shown that the resulting model reduces to the standard diffraction model in the case of PW scattering. These findings unify the treatment of diverse phenomena. For example, neutron scattering in amorphous solids and electron-phonon interaction contributions to electrical transport in perfect crystals are conveniently treated in the context of the generalized diffraction model.

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Furthermore, it has been explicitly demonstrated that many important standard expressions appearing in the literature are obtained as approximations to the diffraction model. Thus, the diffraction model origins of the standard expressions are revealed and the nature of the implicit approximations in the standard forms is clarified.

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